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STUDIES IN QUALITY IMPROVEMENT II: AN ANALYSIS FOR UNREPLICATED FRACTIONAL FACTORIALS

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ABSTRACT

In industrial experimentation it is frequently true that a large proportion of process variation is associated with a small proportion of the process variables. In such circumstances of "effect sparsity" unreplicated fractional designs have frequently been effective in isolating preponderant factors. A very useful graphical analysis for such experiments due to Cuthbert Daniel (1959) employs normal probability plotting. A more formal analysis is presented here which might be used to supplement such plots.

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SIGNIFICANCE AND EXPLANATION

Unreplicated fractional factorial designs are frequently employed as screening designs when it is believed that a condition of effect sparsity will ensure that only a few of the possible effects are likely to be large. A Bayesian analysis is proposed to supplement the graphical technique currently employed for analysis of fractional factorials. In the proposed analysis, the posterior probability that each orthogonal contrast measures a real effect is computed. Sensitivity of the analysis to the assumed frequency and size of large effects is explored through several examples.

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1. INTRODUCTION

The possible importance of fractional factorial designs in industrial applications seems to have been first recognized some 50 years ago (Tippett (1934), see also Fisher (1966) p. 88). Tippett successfully employed a 125th fraction of a 5^5 factorial as a screening design to discover the cause of difficulties in a cotton spinning machine. A general theory for fractional factorial designs was worked out by Finney (1945) and Rao (1947) and other orthogonal arrays which were not, in general, fractional factorials, were introduced by Plackett and Burman (1946). These designs produce confounding of effects of various orders but, as in Tippett's application, their industrial use (see also, for example, Davies (1954); Box and Hunter (1961); Daniel (1959, 1976)) has usually rested on an implicit hypothesis of what we will call <u>effect sparsity</u>. This hypothesis is that in relation to the noise only a small proportion of the effects will be large and the majority will be negligible. The former will be called "active" effects, the remainder "inert" effects. The hypothesis of effect sparsity is associated with the notion that a large proportion of process variation is explained by a small proportion of the process variables. The effect sparsity hypothesis has implications both for <u>design</u> and <u>analysis</u>.

Concerning the design aspect, consider, for example, an experimenter who desired to screen eight factors at two levels, believing that not more than three would be active. He might choose to employ a sixteenth replicate of a 2^8 design of resolution four. This 2^{8-4}_{IV} design has the property that every one of its $\binom{8}{3} = 56$ projections into three-space is a duplicated 2^3

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factorial. Its use would thus ensure that the design provided a duplicated 2^3 factorial in any set of three variables that happened to be active. Obviously such applications employ some guesswork concerning the likely degree of effect sparsity. However, in the situation where experimentation is sequential, a fractional design may be regarded potentially as a first building block in a process of sequential assembly (Box (1982)). Thus, where necessary, additional runs or additional fractions may be combined with the original design to resolve ambiguities (see for example, Box and Hunter (1961); Box, Hunter and Hunter (1978)).

The analysis of fractional factorials and other design arrays can be thought of as involving two distinct stages. In the first stage we attempt to identify certain contrasts which are unlikely to be due to noise and hence deserve interpretation. In the second stage we attempt to associate these contrasts which are believed to be active with specific factors and interactions between factors. Thus in the analysis of a 2-level fractional factorial involving factors A,B,C and D a particular contrast identified as unlikely to be explained by noise might estimate an aliased combination of interactions such as (AB + CD). In practice the ambiguity posed by the apparent activity of such an "alias string" must usually be resolved by further experimentation or occasionally and more dubiously by an appeal to technical knowledge. In this paper we are concerned only with the first problem, that of attempting to identify active contrasts. In what follows we refer to the mean value of an active contrast as an "effect" bearing in mind that depending on how complicated is the model that we have in mind such an effect may correspond with an alias string.

Some of the techniques which have been employed to identify active effects are as follows.

When an estimate of the experimental error variance is available from relevant genuinely replicated runs from current or past experimentation, subject to allowance for selection of the largest contrasts, analysis of variance techniques may be used to judge the reality of estimated effects.

For unreplicated experiments, contrasts associated with supposedly inert higher-order interactions are often used to estimate error variance. This method is however sometimes unsatisfactory because the required inert contrasts may be difficult or impossible to identify.

An even less satisfactory procedure for estimating the experimental error variance employs successive pooling of supposedly nonsignificant components.

A very useful graphical technique due to Daniel (1959) has the advantages that it does not require prior identification of inert contrasts and allows for selection automatically. In this method the empirical cumulative distribution of the estimated effects is plotted on normal probability paper. In the circumstance of effect sparsity, inert effects tend to fall roughly along a straight line through the origin while active effects tend to appear as extreme points falling off the line.

The purpose of the present paper is to present a more formal analysis appropriate to the circumstance of effect sparsity. We advance this as a possibly useful adjunct to the graphical procedures. Plotting is always valuable and in particular can suggest model inadequacies (see Daniel (1959)).

2. AN ANALYSIS FOR UNREPLICATED DESIGNS

Suppose that an effect τ_i $(i = 1,\ldots,\nu)$ is active with probability α, and the active τ_i are i.i.d. $N(0,\sigma_\tau^2)$. Let $T = (T_1,\ldots,T_\nu)$ be the ν estimated effects obtained in the usual way from some orthogonal array and where necessary, standardized so that, given $\underset{\sim}{\tau}$, they all have the same (unknown) variance σ^2. That is, for an inert effect, $T_i = e_i$; for an active effect, $T_i = \tau_i + e_i$; and the error terms e_i are i.i.d. $N(0,\sigma^2)$. If we let $k^2 = (\sigma^2 + \sigma_\tau^2)/\sigma^2$, then $T_1,\ldots,T_\nu$ are i.i.d. from the scale-contaminated normal distribution denoted by $(1 - \alpha)N(0,\sigma^2) + \alpha N(0,k^2\sigma^2)$.

Let $a_{(r)}$ be the event that a particular set of r of the ν effects are active, and let $T_{(r)}$ be the vector of estimated effects corresponding to active effects of $a_{(r)}$. Ther (Box and Tiao, 1968), with $p(\log \sigma)$ locally uniform, the posterior probability that $T_{(r)}$ comprises the active effects is

$$p(a_{(r)}|T,\alpha,k) \propto \left[\frac{\alpha k^{-1}}{1 - \alpha}\right]^r \left[1 - \phi f_{(r)}\right]^{-\nu/2} \tag{1}$$

where $\phi = 1 - \dfrac{1}{k^2} = \dfrac{\sigma_\tau^2}{\sigma^2 + \sigma_\tau^2}$ and $f_{(r)} = T'_{(r)}T_{(r)}/T'T$ is the fraction of the sum of squares associated with $T_{(r)}$.

2.1 The Probability That An Effect Is Active

In particular, the marginal probability p_i that an effect i is active given T, α and k is

$$p_i = \sum_{(r):i \text{ active}} p(a_{(r)}|T,\alpha,k) \ . \tag{2}$$

In general, to compute p_i for $i = 1,\ldots,\nu$, the probabilities (1) must be computed for all 2^ν possible events $a_{(r)}$.

3. CHOOSING α and k

The above analysis makes use of parameters α and k, with α the prior probability of an active effect and k the inflation factor of the standard deviation produced by an active effect. To define a working range for α and k, we have examined the results of several unreplicated fractional factorials. For each example, an estimate of α was obtained as the proportion of effects declared significant by the author(s) of that particular example, and k^2 was estimated by the ratio of the mean squared significant effect over the mean squared inert effect. These values are presented in Table 1. The estimated values of α range between .13 and .27 with an average of about .20. Estimated values of k vary widely between 2.7 and 18 with an average of about 10.

The possibility of bias introduced by restricting attention to published examples and by estimating α and k in this informal manner is recognized. However, we show later that the conclusions to be drawn from our analysis are usually insensitive to moderate changes in α and k and we believe that little would be gained by attempting to be more precise.

TABLE 1.

Estimated values of α and k from published examples of 16 and 32 run two final designs taken from Box, Hunter and Hunter (1978), Davies ed. (1954), Daniel (1976), Bennett and Franklin (1954), Johnson and Leone (1964), and Taguchi and Wu (1980). In Daniel's example the analysis is conducted after making a log transformation in the response.

BHH p. 398	16	.20	7.9
BHH p.327	16	.27	13.9
BHH p. 378	32	.16	11.0
Davies p. 274	16	.13	2.7
Davies p. 462	16	.27	7.1
Daniel p. 71	16	.20	13.0
BF p. 557	16	.27	18.0
JL p. 183	32	.13	3.2
JL p. 196	16	.27	9.5
Taguchi p. 69	16	.13	9.7

4. SOME EXAMPLES

To illustrate the procedure we reanalyze four sets of data from various sixteen-run two-level experiments which have appeared in the literature. In each case the purpose of the analysis is to identify, on the hypothesis of effect sparsity, which columns of the design are associated with effects unlikely to be due to noise. Data from the four examples, labelled I, II, III and IV, are presented in Table 2, which shows the experimental factors, the responses, the column allocations to the 16×16 factorial array, and the estimated effects.

In Figure 1 posterior probability plots are shown on the left and Daniel's normal plots are shown on the right for each of the four examples. For the posterior plots the numbers 1,2,...,15 on the horizontal scale refer to the columns of the design. The solid ~~horizontal~~ vertical lines are posterior probabilities, calculated from equation (2) with $\alpha = 0.2$, $k = 10$. The line on the number i is the probability that the i^{th} column is associated with an active contrast (whether arising from a single effect or from a linear combination of effects corresponding to an alias string). The vertical line on the number zero refers to the probability that there are no active contrasts. The boxes on each line indicate the range of these probabilities when α is varied over the range $0.1 < \alpha < 0.3$ and k is varied over the range $5 < k < 15$. For the normal plots on the right the horizontal scale shows estimated effects and the vertical scale shows the normal score, and each point is labelled with its associated column number.

Examples I, II, and III

(i) For examples I, II and III, consider first the probabilities obtained by setting $\alpha = 0.2$ and $k = 10$ shown by the solid lines. Most of these probabilities are either rather small or else close to unity. This

TABLE 2. DATA FROM FOUR 16-RUN TWO-LEVEL EXPERIMENTS

Example	Source	Design
I	Daniel (1976)	2^4
II	Taguchi and Wu (1980)	2^{9-5}_{III}
III	Box, Hunter and Hunter (1978)	2^{8-4}_{IV}
IV	Davies (1954)	2^4

	Factors	Response
I	Load (A) Flow (B) Speed (C) Mud (D)	Log drill advance
II	Rods (A) Period (B) Material (C) Thickness (D) Angle (E) Opening (F) Current (G) Method (H) Preheating (J)	Tensile strength
III	Temperature (T) Moisture (M) Holding pressure (H) Thickness (V) Booster pressure (B) Cycle time (C) Gate size (G) Speed (S)	Shrinkage
IV	Acid strength (A) Time (B) Amount of acid (C) Temperature (D)	Yield of isatin

Column allocation

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	Response I	II	III	IV
I		A	B		C				D											
II		D	H		G	-F			A	-E				J	B	-C				
III									-S	-T	-M	-V	-H	-B	-C	-G				
IV		A	B		C				D											
Run																				
1	+	-	-	+	-	+	+	-	-	+	+	-	+	-	-	+	.23	43.7	14.0	.08
2	+	+	-	-	-	-	+	+	-	-	+	+	+	+	-	-	.30	40.2	16.8	.04
3	+	-	+	-	-	+	-	+	-	+	-	+	+	-	+	-	.52	42.4	15.0	.53
4	+	+	+	+	-	-	-	-	-	-	-	-	+	+	+	+	.54	44.7	15.4	.43
5	+	-	-	+	+	-	-	+	-	+	+	-	-	+	+	-	.70	42.4	27.6	.31
6	+	+	-	-	+	+	-	-	-	-	+	+	-	-	+	+	.76	45.9	24.0	.09
7	+	-	+	-	+	-	+	-	-	+	-	+	-	+	-	+	1.00	42.2	27.4	.12
8	+	-	+	+	+	+	+	+	-	-	-	-	-	-	-	-	.96	40.6	22.6	.36
9	+	-	-	+	-	+	+	-	+	-	-	+	-	+	+	-	.32	42.4	22.3	.79
10	+	+	-	-	-	-	+	+	+	+	-	-	-	-	+	+	.39	45.5	17.1	.68
11	+	-	+	-	-	+	-	+	+	-	+	-	-	+	-	+	.61	43.6	21.5	.73
12	+	+	+	+	-	-	-	-	+	+	+	+	-	-	-	-	.66	40.6	17.5	.08
13	+	-	-	+	+	-	-	+	+	-	-	+	+	-	-	+	.89	44.0	15.9	.77
14	+	+	-	-	+	+	-	-	+	+	-	-	+	+	-	-	.97	40.2	21.9	.38
15	+	-	+	-	+	-	+	-	+	-	+	-	+	-	+	-	1.07	42.5	16.7	.49
16	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	1.21	46.5	20.3	.23

Effects

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
I	[illegible]	.06	.25	-.01	.50	.00	-.02	.00	.14	.03	-.01	.02	.04	.02	.01	.02
II	43.0	.13	-.15	.30	.15	.40	-.03	.37	.4	-.05	.42	.13	.13	-.37	2.15	3.10
III	19.8	-.6	-.4	-.6	4.6	.9	-.2	-.3	-1.2	.7	.1	.3	-5.5	3.8	.1	-.6
IV	6.4	-.19	-.02	.00	-.08	.03	-.07	.15	.27	-.16	-.25	-.10	-.03	-.01	.12	.02

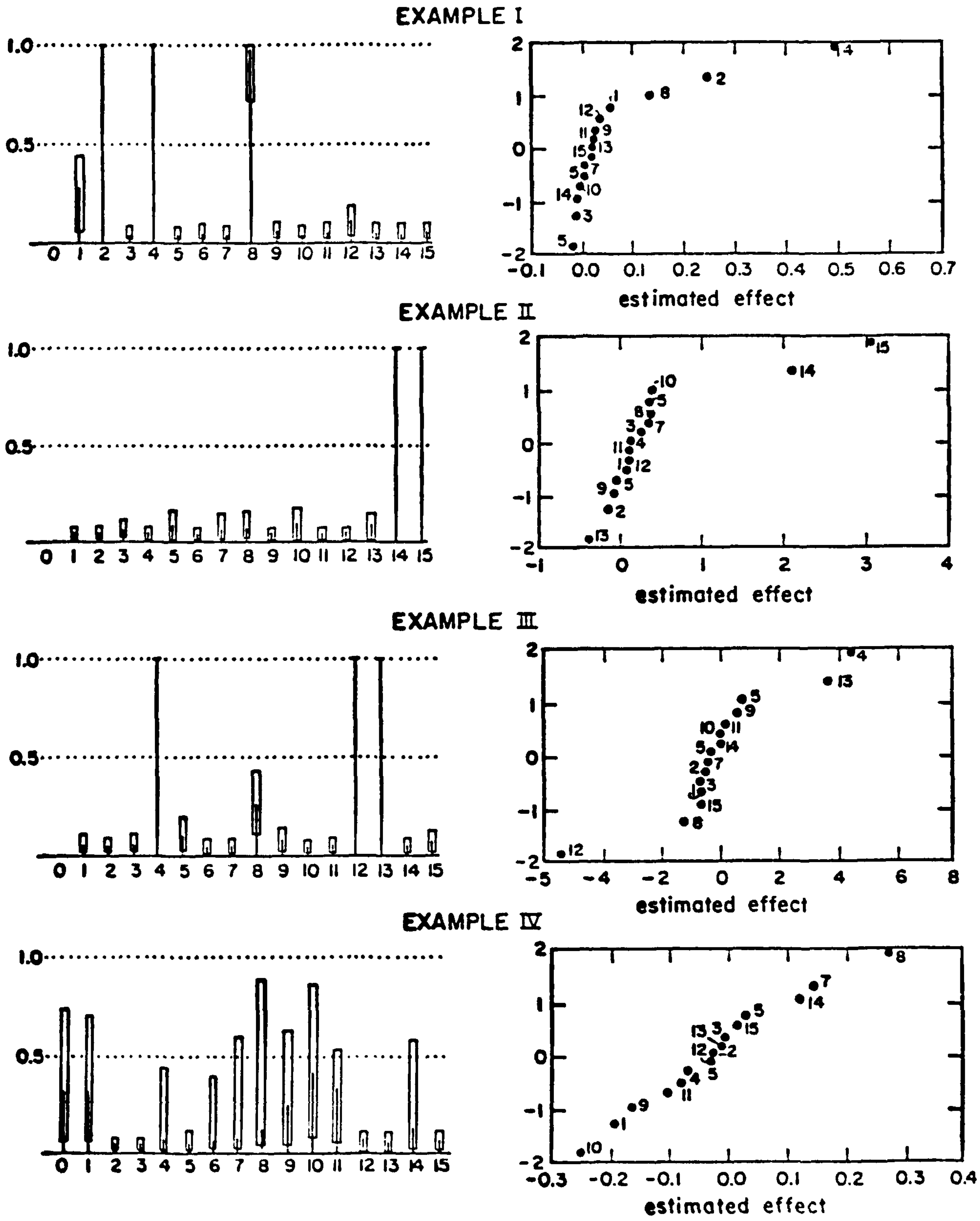

Figure 1. On the left are posterior probability plots for $\alpha = 0.2$, $k = 10$. Boxes show ranges of probabilities over $0.1 < \alpha < 0.3$, $5 < k < 15$. On the right are corresponding normal probability plots.

TSR #2797: Figure 1, page 8, normal plot for Example IV: the positive contrast labelled 5 should be labelled 6.

suggests a division into "inert" and "active" contrasts which seems to agree well with the conclusions of the original authors and with a common sense inspection of the normal plots.

(ii) For each of these examples the probability of no active contrasts is very small over the whole tested range of α and k. The changes (indicated by boxes) that occur in the large probabilities and in the rather small probabilities when α and k are each varied by factors of three, as above, are usually rather small and not such as to change the conclusions about active and inert effects. However larger variations occur for intermediate probabilities (see, for example, contrast 1 in example I and contrast 8 in example III) but again these are not such as to affect the general conclusions and we discuss these further below.

Thus we should tentatively identify as associated with active contrasts:

example I: columns 2, 4 and, somewhat less certainly, 8

example II: columns 14 and 15

example III: columns 4, 12 and 13.

Example IV

This example has been chosen to illustrate what might be seen as a more troublesome situation. The original authors concluded by somewhat dubious use of the analysis of variance that columns 8 and 10 are associated with active contrasts. Our analysis with $\alpha = 0.2$ and $k = 10$ suggests the primary possibility of no activity at all or an extremely weak suggestion of activity for columns 8 and 10. Variation of α and k shows that for this particular set of data the probabilities are much more sensitive, particularly to changes in α. To allow more detailed study analyses are shown in Figure 2 for all combinations of $\alpha = (0.1, 0.2, 0.3)$ and $k = (5, 10, 15)$. In particular it will be seen that for $\alpha = 0.1$, $k = 15$ there is a rather high probability

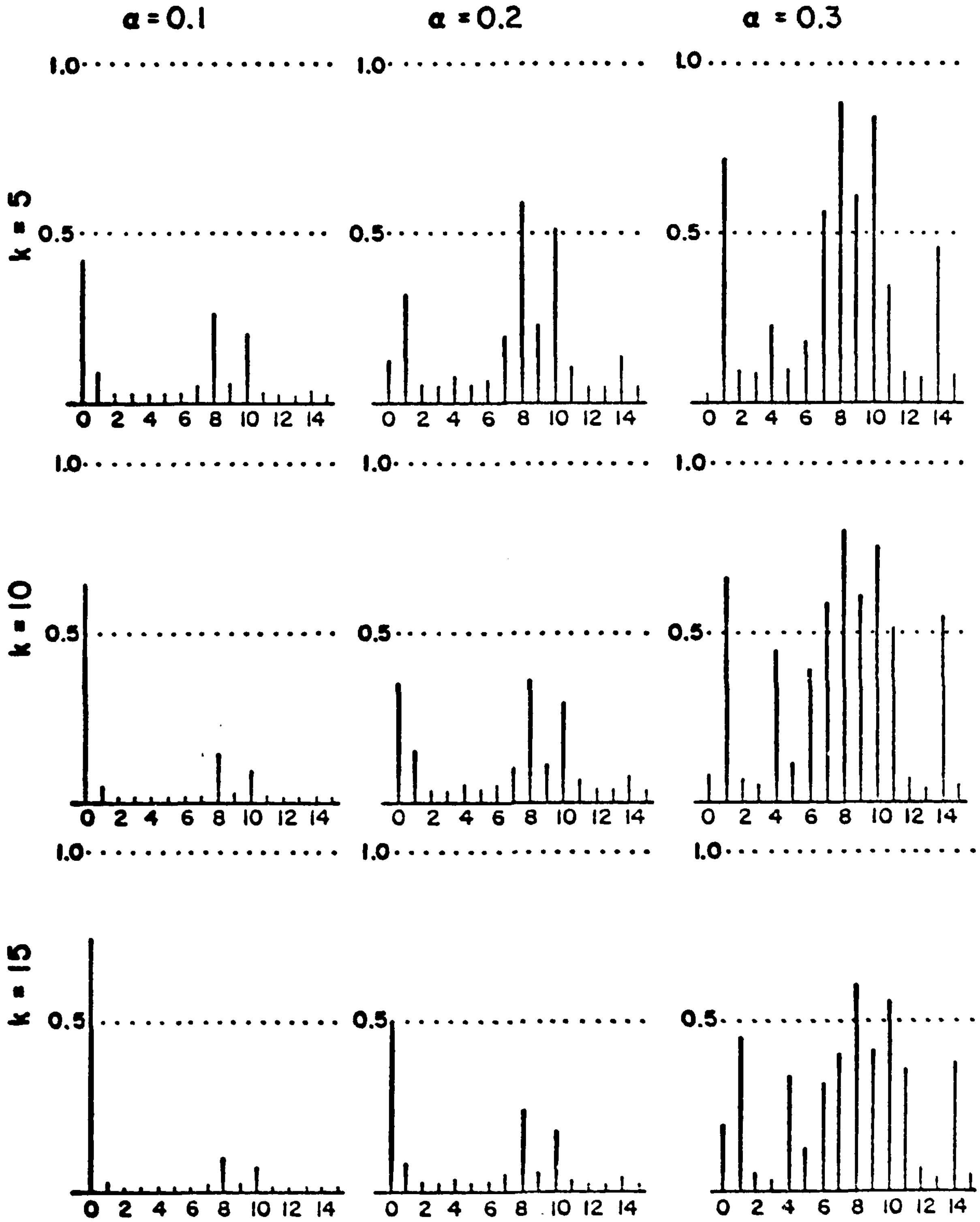

Figure 2. Example IV. Posterior probability plots for all combinations of $\alpha = (0.1, 0.2, 0.3)$ and $k = (5, 10, 15)$.

that no contrast is active. On the other hand for $\alpha = 0.3$, $k = 10$ this probability is small as the column contrasts 1, 7, 8, 9, 10, 11 and 14 all have posterior probabilities greater than 50%. The situation can be further understood by studying the normal plot for this example (Figure 1). On the one hand we can imagine drawing the "error line" through all the points and thus associate all the contrasts with noise, on the other a line might be drawn through the center group (say 4, 6, 12, 2, 13, 3, 15, 5) and the remainder, which are precisely the effects mentioned above, would then be regarded as falling off the line.

We feel that for this example appropriate conclusions are as follows:

(i) It is impossible on the evidence of these data alone to draw reliable inferences about active and inert contrasts: that is, to make inferences which do not change under differing plausible model assumptions.

(ii) It is possible that certain active effects occur, particularly those associated with some or all of columns 1, 7, 8, 9, and 10. If the effects of the corresponding factors, of a size not ruled out by this experiment, were of potential interest and the situation was sequential then further experiments should be run to check out these possibilities. In these further experiments

(a) some or all of the design points might be replicated. This would simultaneously provide greater precision of the estimated effects and an independent estimate of experimental error.

(b) some experiments might be run in which some or all of the ranges of factor levels were widened.

The analysis of these data illustrates a point made by George Barnard (Box (1980) discussion p. 404) that there exist robust and non-robust data samples. That is to say, for certain sets of data, analyses ranging over a wide range of plausible assumptions lead to essentially the same conclusions, while for other sets of data such conclusions are highly sensitive to assumptions. Thus with the robust data of examples I, II and II variation of α and k covering a wide range of plausible assumptions produces little change in the conclusions. However with the non-robust data of example IV the conclusions are much more sensitive to the assumptions.

An important part of modern statistical analysis made available by the computer is aimed at revealing the state of robustness that occurs in any given situation. At least for moderate sample sizes (such as $n = 16$) the posterior probability calculations discussed here can be made rapidly to provide visual displays of probability plots such as those in Figures 1-2 and their sensitivity to changes in α and k can be readily explored. Such sensitivity analysis enables one to decide whether reasonably reliable conclusions are possible from present data or whether further experimentation is needed.

5. DISTRIBUTION OF THE EFFECTS τ

It is possible also, for given α and k, to obtain the posterior distribution for each effect τ_i as a weighted sum of 2^{n-2} t-distributions together with mass $1 - p_i$ at zero (see Appendix).

For the demonstrably active effects, $1 - p_i$ will be close to zero and the weighted sums of t-distributions would in particular provide Bayesian intervals for these effects. Calculation of the complete posterior distribution is cumbersome although it is well approximated in most cases by summing those t-distributions with relatively large weights. Alternately for many purposes the mean and standard deviation of the posterior distribution would be adequate and these are more conveniently obtained.

APPENDIX

To obtain the posterior distribution of $\tau_{(r)}$, given $a_{(r)}$, write

$$p(T|a_{(r)},\tau_{(r)},\sigma)$$

$$\propto \sigma^{-\nu}\exp\{-\frac{1}{2\sigma^2}[(T_{(r)}-\tau_{(r)})'(T_{(r)}-\tau_{(r)})+T'T-T'_{(r)}T_{(r)}]\}$$

$$p(\tau_{(r)}|a_{(r)},\sigma,k) \propto (k^2-1)^{-r/2}\sigma^{-r}\exp\{-\frac{1}{2\sigma^2}(\frac{1}{k^2-1})\tau'_{(r)}\tau_{(r)}\}$$

$$p(\sigma) \propto \frac{1}{\sigma}$$

to give

$$p(\tau_{(r)},|a_{(r)},T,k) \propto \int_0^\infty (k^2-1)^{-r/2}\sigma^{-\nu-r-1}\exp\{-\frac{1}{2\sigma^2}\cdot$$

$$[(T_{(r)}-\tau_{(r)})'(T_{(r)}-\tau_{(r)})+T'T-T'_{(r)}T_{(r)}+\frac{1}{k^2-1}\tau'_{(r)}\tau_{(r)}]\}d\sigma$$

$$\propto (k^2-1)^{-r/2}[(T_{(r)}-\tau_{(r)})'(T_{(r)}-\tau_{(r)})+$$

$$+T'T-T'_{(r)}T_{(r)}T_{(r)}+\frac{1}{k^2-1}\tau'_{(r)}\tau_{(r)}]^{\frac{-(\nu+r)}{2}}.$$

This can be rewritten to give

$$p(\tau_{(r)}|a_{(r)},T,k) \propto [1+\frac{(\tau_{(r)}-\phi T_{(r)})'(\tau_{(r)}-\phi T_{(r)})}{\phi(T'T-\phi T'_{(r)}T_{(r)})}]^{\frac{-(\nu+r)}{2}}$$

which implies the posterior distribution of $\tau_{(r)}$, given $a_{(r)}$, is multivariate t with ν degrees of freedom, mean $\phi T_{(r)}$ dispersion matrix $\frac{\phi}{\nu}(T'T-\phi T'_{(r)}T_{(r)})I$. In particular, if $s^2_{(r)} = \frac{\phi}{\nu}(T'T-\phi T'_{(r)}T_{(r)})$, then under $a_{(r)}$ each of

$$t = \frac{\tau_i - \phi T_i}{s_{(r)}}$$

is distributed t_ν for $i \in (r)$.

The complete posterior distribution of τ_i is then given by (see, e.g., Box and Tiao (1968)),

$$p(\tau_i|y,\alpha,k) = \sum_{(r)} p(\tau_i|y,\alpha,k,a_{(r)})p(a_{(r)}|y,\alpha,k)$$

$$= (1 - p_i)I_{[\tau_i=0]} + \sum_{(r):i \text{ active}} p(\tau_i|y,\alpha,k,a_{(r)})p(a_{(r)}|y,\alpha,k) .$$

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

In industrial experimentation it is frequently true that a large proportion of process variation is associated with a small proportion of the process variables. In such circumstances of "effect sparsity" unreplicated fractional designs have frequently been effective in isolating preponderant factors. A very useful graphical analysis for such experiments due to Cuthbert Daniel (1959) employs normal probability plotting. A more formal analysis is presented here which might be used to supplement such plots.